

Tunneling Hamiltonian

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Abstract. For the description of the transport of electrons across a quantum dot, which is tunnel coupled to leads at different chemical potentials, it is usual to assume that the total Hamiltonian of the composite system of the leads and the quantum dot is the sum of three contributions: That of the leads (noninteracting electrons), that of the quantum dot and a third one, the “tunneling Hamiltonian”, which reflects the possibility that electrons can move from the leads to the quantum dot or vice versa. The text aims at a mathematically clear derivation of such a separation. I will start the discussion with the total Hamiltonian of the system acting on a many-electron wave function, including the attractive interaction between nuclei and electrons as well as the repulsive Coulomb-interaction between different electrons. Indeed, a natural separation of the total Hamiltonian in the described form will be obtained. An analysis of the tunneling Hamiltonian shows that the electron-electron interaction yields contributions to it which represent the correlated tunneling of *two* electrons at the same time. For the derivations it was useful to introduce a map called “antisymmetric product”. In an appendix I show possible exact representations of the total Hamiltonian (with arbitrary potential $V(r)$) obtained by the use of the antisymmetric product.

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1. Hamilton operator

The Hamilton operator of a crystal acts on an N -electron wave function

$$\psi : D^N \rightarrow \mathbb{C}, \quad (1)$$

where $D = \mathbb{R}^3 \times \{\uparrow, \downarrow\}$, $D^N = D \times D \times \dots \times D$. It contains the kinetic energy, the attractive force between the nuclei and the electrons and the repulsion between different electrons. It can be written as

$$H\psi = -\frac{\hbar^2}{2m}\Delta\psi + \sum_{i=1}^N V(r_i)\psi + \sum_{i<j} \frac{e^2}{|r_i - r_j|}\psi. \quad (2)$$

The position of the nuclei is considered as constant in time within this equation [1]. I summarized in “ $V(r)$ ” the potentials of the bare nuclei located at the lattice points of the crystal. A wave function as in (1) can be viewed as a set of 2^N maps

$$\begin{aligned} \psi_{\sigma_1, \dots, \sigma_N} : (\mathbb{R}^3)^N &\rightarrow \mathbb{C}, \\ (r_1, \dots, r_N) &\rightarrow \psi_{\sigma_1, \dots, \sigma_N}(r_1, \dots, r_N). \end{aligned}$$

The Hamiltonian leaves the spin-variables $\sigma_i \in \{\uparrow, \downarrow\}$ unchanged and acts on each of the 2^N components.

The above shape of the Hamilton operator is quite general. It should be valid even if the nuclei are not located at the points of a regular lattice and also, for example, if one considers two finite crystals separated by vacuum. The changes enter into the potential $V(r)$.

Later on in the text it will turn out to be convenient to have an extra notation for the contribution of the electron-electron repulsion to the total Hamiltonian. I define thus

$$H^{(int)}\psi = \sum_{i<j} \frac{e^2}{|r_i - r_j|}\psi. \quad (3)$$

2. Antisymmetric wave functions

2.1. Slater determinants

A wave function of N fermions is required to be antisymmetric. Slater determinants [1] provide a way to construct antisymmetric wave functions of N electrons by the use of one-electron wave functions: For a system of one-electron wave functions $\psi_i : D \rightarrow \mathbb{C}, i = 1, \dots, N$, one can define

$$\psi_1 \otimes \dots \otimes \psi_N : D^N \rightarrow \mathbb{C}$$

as

$$\psi_1 \otimes \dots \otimes \psi_N(x_1, \dots, x_N) := \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \text{sgn}(\pi) \psi_{\pi(1)}(x_1) \dots \psi_{\pi(N)}(x_N).$$

I used “ x_i ” to denote elements of D , “ S_N ” is the set of all permutations of the set $\{1, \dots, N\}$.

(For the set of permutations of any finite set the following rules hold: Any permutation can be represented as a product of subsequent “transpositions”. These are those special permutations which exchange only two elements and act, apart from this, as identity. The representation of an arbitrary permutation as product of transpositions is not unique, but the property “even“ or “odd” of the number of needed transpositions is. Therefore, one can assign a sign to the permutation, $\text{sgn}(\pi) = \pm 1$, in case the number is even/odd. This sign is multiplicative, $\text{sgn}(\pi\pi') = \text{sgn}(\pi)\text{sgn}(\pi')$. The “Leibniz formula” uses permutations to express the determinant.)

At any rate, the Slater determinant is an antisymmetric wave function. For any two (quadratically integrable) wave functions $\psi, \psi' : D^N \rightarrow \mathbb{C}$ one defines the scalar product [1] as

$$\langle \psi | \psi' \rangle := \sum_{\sigma_1} \dots \sum_{\sigma_N} \int_{(\mathbb{R}^3)^N} \psi_{\sigma_1, \dots, \sigma_N}^*(r_1, \dots, r_N) \psi'_{\sigma_1, \dots, \sigma_N}(r_1, \dots, r_N).$$

2.2. Normalization condition

The norm is defined by $\| \psi \|^2 = \langle \psi | \psi \rangle$. For simplicity, the prefactor $1/\sqrt{N!}$ was included in the Slater determinant. It ensures that, if the functions ψ_1, \dots, ψ_N form an orthonormal system, then the norm of their Slater determinant is one. To fill the normalization condition with life, I tried to clarify its relation to the particle density. In the case of N distinguishable particles represented by a wave function $\psi(r_1, \sigma_1, \dots, r_N, \sigma_N)$ one could speak about a probability of finding particle 1 with spin σ_1 within a volume $V_1 \subset \mathbb{R}^3$ and ... and particle N with spin σ_N within a volume $V_N \subset \mathbb{R}^3$. The probability might be defined as

$$\int_{V_1} dr_1 \dots \int_{V_N} dr_N |\psi(r_1, \sigma_1, \dots, r_N, \sigma_N)|^2.$$

Correspondingly, one would define the number of particles which can be found in a volume $V \subset \mathbb{R}^3$ as

$$\sum_{\sigma_1, \sigma_2} \left\{ \int_{V \times V^c} + \int_{V^c \times V} + 2 \int_{V \times V} \right\} |\psi_{\sigma_1, \sigma_2}(r_1, r_2)|^2.$$

I assumed the special case $N = 2$ and used the notation $V^c = \mathbb{R}^3 \setminus V$ for this. One can then represent

$$\int_{V \times V^c} + \int_{V^c \times V} + 2 \int_{V \times V} = \int_{V \times \mathbb{R}^3} + \int_{\mathbb{R}^3 \times V}.$$

The way of defining the probability and representing it in an alternative form can be generalized to the case of arbitrary N . If the one-electron wave functions ψ_1, \dots, ψ_N contributing to a Slater determinant form an orthonormal system, then one obtains indeed the particle density

$$\rho(r) = \sum_{i=1}^N \sum_{\sigma} |\psi_i(r, \sigma)|^2$$

which one would expect intuitively.

2.3. Antisymmetric product

A Slater determinant can be viewed as an antisymmetric product of wave functions $\psi_i : D \rightarrow \mathbb{C}$. A generalization is possible: For

$$\psi : D^m \rightarrow \mathbb{C}, \quad \varphi : D^n \rightarrow \mathbb{C}$$

one can define

$$\psi \otimes \varphi : D^{m+n} \rightarrow \mathbb{C}$$

by

$$\begin{aligned} \psi \otimes \varphi(x_1, \dots, x_{m+n}) &:= \sqrt{\frac{m!n!}{(m+n)!}} \sum_{M: M \subset \{1, \dots, m+n\}, |M|=m} \text{sgn}(\pi_M) \\ &\quad \psi(x_{\pi_M(1)}, \dots, x_{\pi_M(m)}) \varphi(x_{\pi_M(m+1)}, \dots, x_{\pi_M(m+n)}). \end{aligned}$$

I used “ $|M|$ ” to denote the number of elements of M . The permutation π_M is the one which counts at first the elements of M in increasing order and then the elements of its complement $M^c := \{1, \dots, m+n\} \setminus M$. More precisely:

$$\pi_M(1) = x_1, \dots, \pi_M(m) = x_m, \pi_M(m+1) = y_1, \dots, \pi_M(m+n) = y_n$$

if $M = \{x_1, \dots, x_m\}$, $M^c = \{y_1, \dots, y_n\}$ in increasing order. By the property $\text{sgn}(\pi_M) \text{sgn}(\pi_{M^c}) = (-1)^{mn}$ one can show the relation

$$\psi \otimes \varphi = (-1)^{mn} \varphi \otimes \psi.$$

If ψ and φ are antisymmetric, then also $\psi \otimes \varphi$. This can be seen by applying the “antisymmetrizer” [5] to ψ and φ .

The product is bilinear and associative:

$$\psi \otimes (\varphi \otimes \lambda) = (\psi \otimes \varphi) \otimes \lambda.$$

A symmetric representation is given by

$$\begin{aligned} &[\psi \otimes (\varphi \otimes \lambda)](x_1, \dots, x_{m+n+l}) = \\ &= \sqrt{\frac{m!n!l!}{(m+n+l)!}} \sum_{M, N, L: \quad M \dot{\cup} N \dot{\cup} L = \{1, \dots, m+n+l\}, |M|=m, |N|=n, |L|=l} \text{sgn}(\pi_{M, N, L}) \\ &\quad \psi(x_{\pi_{M, N, L}(1)}, \dots, x_{\pi_{M, N, L}(m)}) \\ &\quad \varphi(x_{\pi_{M, N, L}(m+1)}, \dots, x_{\pi_{M, N, L}(m+n)}) \\ &\quad \lambda(x_{\pi_{M, N, L}(m+n+1)}, \dots, x_{\pi_{M, N, L}(m+n+l)}), \end{aligned}$$

where $\pi_{M, N, L}$ counts at first the elements of M , then the elements of N , and finally the elements of L in increasing order.

As a consequence, expressions like “ $\psi_1 \otimes \dots \otimes \psi_N$ ” (without any brackets) are well-defined for $\psi_i : D^{m_i} \rightarrow \mathbb{C}$. Indeed, if all $m_i = 1$, then the product is the Slater determinant defined above.

3. Vector space

3.1. Vector space of the leads

About the vector space of the many-electron states of the leads I assume that it is generated by single-electron wave functions via Slater determinants and linear combinations of these. This is in agreement with the concept that the many-electron states in a large crystal can be specified by saying which “one-electron levels” are occupied. The Fermi-Dirac distribution was derived in Ref. [1] by the use of this idea. According to the Born-von Karman boundary condition one has two such one-electron wave functions for every “allowed” wave vector k in a primitive cell of the reciprocal lattice. I denote the one-electron wave functions by

$$\begin{aligned} \psi_{lk\sigma} : \mathbb{R}^3 \times \{\uparrow, \downarrow\} &\rightarrow \mathbb{C} \\ (r, \sigma') &\mapsto \psi_{lk}(r) \delta_{\sigma}(\sigma'). \end{aligned}$$

The index “ l ” denotes the lead, $\psi_{lk}(r)$ is a Bloch wave function depending only on a space-variable. A further band index might be included but is not essential to the purpose of this work. The number of one-electron levels is proportional to the size of the crystal [1]. The $\psi_{lk\sigma}$ form an orthonormal system in the quadratically integrable functions $D \rightarrow \mathbb{C}$. For every natural number $n \leq |R|$ one can define

$$V_n(R) := \text{lin} \{ \psi_1 \otimes \dots \otimes \psi_n : \psi_1, \dots, \psi_n \in R \}.$$

(With “ $\text{lin}(S)$ ” I denote the set of all linear combinations of elements in S .) $V_n(R)$ is a linear subspace of the set of all antisymmetric and quadratically integrable maps $D^n \rightarrow \mathbb{C}$. The subsets $M \subset R$ with $|M| = n$ form an orthonormal basis of $V_n(R)$ via an identification

$$M = \psi_1 \otimes \dots \otimes \psi_n, \text{ where } \psi_1, \dots, \psi_n$$

is a list of the elements of M in some previously chosen and fixed order. The set of linear combinations of Slater determinants is really larger than the set of Slater determinants. In general, the solutions to the eigenvalue equation $H\psi = E\psi$ are linear combinations of an infinite number of Slater determinants. Any antisymmetric function can be approximated by a sequence of linear combinations of Slater determinants [5], while there is in general no way to approximate a linear combination of Slater determinants by a sequence of Slater determinants. The ground state energies of two-electron atoms have been calculated numerically by the use of the Hamilton operator, Eq. (2) [5]. The good quantitative agreement with experiments indicates that this rather intransparent Hamiltonian is indeed the right one as long as relativistic effects are ignored. Moreover, the Hartree-Fock equations have been derived from this Hamiltonian. They contain an *exchange term* which has been made responsible e.g. for screening effects.

Essentially in analogy to Ref. [3] I define the vector space $V(R)$ as

$$V(R) := V_0(R) \times V_1(R) \times \dots \times V_{|R|}(R),$$

where $V_0(R) := \mathbb{C}$. Since the $V_n(R)$ are Hilbert spaces via their scalar products $\langle \cdot | \cdot \rangle$, $V(R)$ is also a Hilbert space. $V_n(R)$ can be viewed as a subset of $V(R)$ by the identification

$$\psi \in V_n(R) \quad \text{corresponds to} \quad (0, \dots, 0, \psi, 0, \dots, 0) \in V(R).$$

The element $(\psi_0, \dots, \psi_{|R|}) \in V(R)$ can be written as $\psi_0 + \dots + \psi_{|R|}$. The scalar product is

$$\langle (\psi_0, \dots, \psi_{|R|}) | (\varphi_0, \dots, \varphi_{|R|}) \rangle = \sum_{i=0}^{|R|} \langle \psi_i | \varphi_i \rangle.$$

Moreover, one has the map

$$\begin{aligned} \otimes : V(R) \times V(R) &\rightarrow V(R) \\ ((\psi_0, \dots, \psi_{|R|}), (\varphi_0, \dots, \varphi_{|R|})) &\mapsto \sum_{i,j: i+j \leq |R|} \psi_i \otimes \varphi_j. \end{aligned}$$

The elements of $V(R)$ can be viewed as linear combinations of subsets of R , in the same way as the elements of $V_n(R)$ can be viewed as such linear combinations. The element $1 \in \mathbb{C} = V_0(R)$ represents the empty set. With this interpretation one can write for $M, N \subset R$:

$$M \otimes N = \pm M \cup N \quad \text{in case } M \cap N = \emptyset$$

and zero otherwise.

3.2. Approximate Hamiltonian

The Hamiltonian “ H^R ” of the reservoirs is given by Eq. (2) in case one replaces the potential $V(r)$ appearing there by the potential of the reservoirs “ $V^R(r)$ ”. ($V(r) = V^R(r) + V^Q(r)$ with $V^Q(r)$ the potential which enters the Hamiltonian of the quantum dot.) There is little hope that H^R is indeed an endomorphism of the Hilbert space $V(R)$, i.e., in general the image $H^R(V(R))$ is not a subset of $V(R)$. However, I assume that for states $\psi \in V(R)$ with “sensible” electron numbers $H^R\psi$ is very close to being an element of $V(R)$ and that in this sense $V(R)$ is a good choice of the vector space on which the Hamiltonian operates. By the use of the orthogonal projection

$$p_{V(R)} : \quad \text{lin}(V(R) \cup H^R(V(R))) \rightarrow V(R),$$

which can be defined by the condition

$$\psi - p_{V(R)}\psi \perp V(R),$$

one obtains the approximate Hamiltonian $p_{V(R)}H^R$. This is indeed a hermitian operator $V(R) \rightarrow V(R)$ and defines the mathematical model of the reservoirs.

3.3. Vector space of the composite system

The construction of a vector space $V(M)$ can be realized for any finite set M of one-electron wave functions. In case M is an orthonormal system the subsets of M form an orthonormal basis of $V(M)$. I assume that the vector space of the many-electron states of the isolated quantum dot is given by $V(Q)$ where Q is a finite orthonormal system of one-electron wave functions. Analogously to the above arguments, I assume that for the “most relevant” states φ of the quantum dot $H^Q\varphi$ is very close to being an element in $V(Q)$. Hence, a good approximate Hamiltonian might be $p_{V(Q)}H^Q$.

I feel forced to assume that $R \cup Q$ is still an orthonormal system. This assumption is in agreement with previous tunneling theories [7]. Going even beyond this, I demand that

$$\begin{aligned} H^R(V(R)) &\subset \overline{V(Q^\perp)}, \\ H^Q(V(Q)) &\subset \overline{V(R^\perp)}. \end{aligned} \quad (4)$$

“ R^\perp ” is the orthogonal complement of R in the square-integrable functions $D \rightarrow \mathbb{C}$. $V(R^\perp)$ is the set of all linear combinations of Slater determinants of elements in R^\perp , in the same way as $V(R)$ is the set of all linear combinations of Slater determinants of elements in R . Finally, $\overline{V(R^\perp)}$ is the topological closure of $V(R^\perp)$, i.e., the set of all infinite and convergent linear combinations of Slater determinants of elements in R^\perp . The demand is that, in case one applies the Hamiltonian of the reservoirs to any wave function in the chosen vector space of the leads, then the result is a wave function for whose representation as an (infinite) linear combination of Slater determinants of one-electron wave functions exclusively elements in Q^\perp are needed, and vice versa. This should be approximately fulfilled if the distance between the sub-systems is large.

(Remark: $V(R)$ and $V(R^\perp)$ are not orthogonal since \mathbb{C} is contained in both of them. Still, they are somehow antisymmetric complements since for all $\psi \in V(R), \varphi \in V(R^\perp) : \|\psi \otimes \varphi\|^2 = \|\psi\|^2 \|\varphi\|^2$. One might take this equation as a definition of an antisymmetric complement “a.c.” and think about the question whether indeed $V(R)^{a.c.} = \overline{V(R^\perp)}$.)

As vector space of the many-electron states of the composite system of reservoirs and quantum dot $V(R \cup Q)$ should serve. In case of large distance between the two systems the assumption makes sense, for sure: The eigenstates of the composite system can be expected to be just the product of the eigenstates of the separate systems.

The Hamiltonian, Eq. (2), acts on $V(R \cup Q)$ like

$$H(\psi_0, \psi_1, \dots, \psi_{|R \cup Q|}) = (0, H\psi_1, \dots, H\psi_{|R \cup Q|}),$$

i.e., in particular $H\emptyset = 0$. As the final model Hamiltonian I take

$$p_{V(R \cup Q)}H : V(R \cup Q) \rightarrow V(R \cup Q).$$

The vector space $V(R \cup Q)$ is a realization of the “tensor product” of the vector spaces $V(R)$ and $V(Q)$, which is defined in mathematics in a purely formal way. The antisymmetric product is a realization of the corresponding bilinear map

" $\otimes : V(R) \times V(Q) \rightarrow V(R \cup Q)$ ". The purely formal tensor product has been used in Ref. [2] to construct the vector space of a composite system of two sub-systems.

4. Additive separation of the Hamiltonian

For a start, I want to consider the action of the total Hamiltonian on an antisymmetric product $\psi \otimes \varphi \in V(R \cup Q)$ with $\psi \in V_m(R), \varphi \in V_n(Q), 1 \leq m \leq |R|, 1 \leq n \leq |Q|$. For this I write the electrostatic potential $V(r)$ caused by the nuclei entering the total Hamiltonian, Eq. (2), as $V(r) = V^Q(r) + V^R(r)$ where $V^S(r)$ is the electrostatic potential entering the Hamiltonian of the corresponding sub-system. The product $\psi \otimes \varphi$ can be written as

$$\psi \otimes \varphi = \sqrt{\frac{m!n!}{(m+n)!}} \sum_{M \subset \{1, \dots, m+n\}: |M|=m} \text{sgn}(\pi_M) S_{\pi_M} [\psi * \varphi],$$

where $\psi * \varphi : D^{m+n} \rightarrow \mathbb{C}$ is defined by

$$\psi * \varphi(x_1, \dots, x_{m+n}) = \psi(x_1, \dots, x_m) \varphi(x_{m+1}, \dots, x_{m+n})$$

and where for any permutation $\pi \in S_l, l \in \mathbb{N}$, and any function

$$\alpha : D^l \rightarrow \mathbb{C}$$

the function $S_\pi \alpha : D^l \rightarrow \mathbb{C}$ is given by

$$S_\pi \alpha(x_1, \dots, x_l) = \alpha(x_{\pi(1)}, \dots, x_{\pi(l)}).$$

This representation is convenient since the Hamiltonian commutes with the operators S_π [5],

$$H[\psi \otimes \varphi] = \sqrt{\frac{m!n!}{(m+n)!}} \sum_{M \subset \{1, \dots, m+n\}: |M|=m} \text{sgn}(\pi_M) S_{\pi_M} H[\psi * \varphi].$$

With a little bookkeeping [1] one can write

$$\begin{aligned} H[\psi \otimes \varphi] &= (H^R \psi) \otimes \varphi + \psi \otimes (H^Q \varphi) \\ &+ \sqrt{\frac{m!n!}{(m+n)!}} \sum_{M \subset \{1, \dots, m+n\}: |M|=m} \text{sgn}(\pi_M) S_{\pi_M} T_{m,n} [\psi * \varphi], \end{aligned} \quad (5)$$

where $T_{m,n}$ is defined by

$$\begin{aligned} T_{m,n} &:= T_{m,n}^{(Q)} + T_{m,n}^{(R)} + T_{m,n}^{(int)}, \\ T_{m,n}^{(int)} [\alpha(r_1, \sigma_1, \dots, r_{m+n}, \sigma_{m+n})] &:= \\ &\left\{ \sum_{i=1}^m \sum_{j=m+1}^{m+n} \frac{e^2}{|r_i - r_j|} \right\} \alpha(r_1, \sigma_1, \dots, r_{m+n}, \sigma_{m+n}), \\ T_{m,n}^{(Q)} [\alpha(r_1, \sigma_1, \dots, r_{m+n}, \sigma_{m+n})] &:= \end{aligned}$$

$$\left\{ \sum_{i=1}^m V^Q(r_i) \right\} \alpha(r_1, \sigma_1, \dots, r_{m+n}, \sigma_{m+n}),$$

and where $T_{m,n}^{(R)}$ has the corresponding definition.

For the above alternative representation of $H[\psi \otimes \varphi]$ the assumption $m, n \geq 1$ was made. The equality, however, is correct also in the cases that m or n or both of them are zero. (For example, $\psi \otimes \varphi = \psi\varphi$ in case ψ or φ is only a number; $T_{0,0} = 0$.) Roughly speaking, the terms in $T_{m,n}^{(int)}$ reflect the repulsion between electrons in the contacts on the one hand and electrons in the quantum dot on the other hand. The terms in $T_{m,n}^{(Q)}$ represent the attractive interaction of the electrons in the reservoirs on the one hand and the nuclei in the quantum dot on the other hand.

Since $p_{V(R \cup Q)}H$ was chosen as the model Hamiltonian, the projection $p_{V(R \cup Q)}$ should be applied to both sides of Eq. (5). By the demanded complementarity (4), one obtains the equation

$$\begin{aligned} p_{V(R \cup Q)}H[\psi \otimes \varphi] &= (p_{V(R)}H^R\psi) \otimes \varphi + \psi \otimes (p_{V(Q)}H^Q\varphi) \\ &+ p_{V(R \cup Q)} \sqrt{\frac{m!n!}{(m+n)!}} \sum_{M \subset \{1, \dots, m+n\}: |M|=m} \text{sgn}(\pi_M) S_{\pi_M} T_{m,n}[\psi * \varphi]. \end{aligned}$$

Proof:

I used that $p_{V(R \cup Q)}[(H^R\psi) \otimes \varphi] = (p_{V(R)}H^R\psi) \otimes \varphi$ for any $\psi \in V_m(R), \varphi \in V_n(Q), m, n \geq 0$. Thus, I ought to show that

$$(H^R\psi - p_{V(R)}H^R\psi) \otimes \varphi \perp V(R \cup Q).$$

According to the complementarity-condition (4), $H^R\psi$ is a (maybe infinite) linear combination of Slater determinants of functions in Q^\perp . Since R is a finite subset of Q^\perp , one can assume that all of the Slater determinants appearing in the expansion have the shape

$$\psi_1 \otimes \dots \otimes \psi_{i_0} \otimes \psi_{i_0+1} \otimes \dots \otimes \psi_m,$$

where $\psi_i \in R$ if $i \leq i_0$, $\psi_i \perp R$ otherwise. If one applies the projection $p_{V(R)}$ to such a Slater determinant, then one obtains zero in case $i_0 < m$. The Slater determinant remains unchanged in case $i_0 = m$. Thus, $H^R\psi - p_{V(R)}H^R\psi$ is a linear combination of such determinants with $i_0 < m$. For any $\varphi \in V_n(Q)$ and any such Slater determinant, however, one gets

$$\psi_1 \otimes \dots \otimes \psi_{i_0} \otimes \psi_{i_0+1} \otimes \dots \otimes \psi_m \otimes \varphi \perp V(R \cup Q). \quad \square$$

For any two endomorphisms $A \in \text{End}(V(R)), B \in \text{End}(V(Q))$ ($\text{End}(V)$ is the set of linear maps $V \rightarrow V$) there is a unique well-defined endomorphism " $A \otimes B$ " $\in \text{End}(V(R \cup Q))$ which has the property:

$$A \otimes B(\psi \otimes \varphi) = (A\psi) \otimes (B\varphi) \text{ for all } \psi \in V(R), \varphi \in V(Q).$$

The proof of this statement is straightforward and perfectly analogous to the proof of the corresponding statement about formal tensor products. One can define:

$$\begin{aligned} H_{tot} &:= p_{V(R \cup Q)} H, \\ H_R &:= (p_{V(R)} H^R) \otimes 1_{V(Q)}, \\ H_Q &:= 1_{V(R)} \otimes (p_{V(Q)} H^Q), \end{aligned}$$

and finally

$$H_T := H_{tot} - H_R - H_Q. \quad (6)$$

All of these are hermitian operators on $V(R \cup Q)$.

5. Creation- and annihilation operators

By the use of creation- and annihilation operators [3] H_T can be expressed in a compact form. For any normalized element $\psi \in V_1(R \cup Q)$ one can define the creation operator of ψ as the map

$$\begin{aligned} c_\psi^\dagger &: V(R \cup Q) \rightarrow V(R \cup Q), \\ \varphi &\mapsto \psi \otimes \varphi. \end{aligned}$$

The annihilation operator of the one-electron level ψ is defined as the adjoint operator of the creation operator, $c_\psi := (c_\psi^\dagger)^\dagger$.

6. Expression for H_T in terms of creation- and annihilation operators

So far, a representation of the total Hamiltonian

$$H_{tot} = H_R + H_Q + H_T$$

was obtained, where H_R can be called the contribution of the leads, H_Q is the contribution of the quantum dot and H_T is the tunneling Hamiltonian. The main part of this text aims at a description of H_T . H_T leaves the particle number unchanged, since the other contributions as well as the total Hamiltonian are doing so; $H_T \emptyset = 0$.

For the description of the linear operator H_T one can use any basis of $V(R \cup Q)$. Independently of whether H_R and H_Q are diagonal in the Slater determinants given by the subsets of $R \cup Q$ one can thus use these Slater determinants for the description. For example, if x_1, \dots, x_m are m different elements in R , if y_1, \dots, y_n are n different elements in Q and if $z_1, \dots, z_{m+n} \in R \cup Q$ are $m+n$ different elements, then one obtains according to Eq. (5)

$$\begin{aligned} \langle z_1 \otimes \dots \otimes z_{m+n} | H_T [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle &= \\ \frac{1}{(m+n)!} \sum_{M \subset \{1, \dots, m+n\}; |M|=m} \sum_{\pi \in S_{m+n}} \sum_{\tau \in S_m} \sum_{\eta \in S_n} & \\ sgn(\pi_M) sgn(\pi) sgn(\tau) sgn(\eta) & \\ \langle z_{\pi(1)} * \dots * z_{\pi(m+n)} | & \\ S_{\pi_M} T_{m,n} [x_{\tau(1)} * \dots * x_{\tau(m)} * y_{\eta(1)} * \dots * y_{\eta(n)}] \rangle. & \end{aligned} \quad (7)$$

6.1. Contribution of the electron-electron interaction to H_T

First, the contribution of $T_{m,n}^{(int)}$ to the matrix element is considered. Hence, I assume that $m, n \geq 1$. For any $1 \leq i \leq m, 1 \leq j \leq n$, the permutation $k_{ij} \in S_{m+n}$ is defined by (myself and) the conditions:

- $\kappa_{ij}(1) = i, \kappa_{ij}(2) = j$.
- $\kappa_{ij}(3), \dots, \kappa_{ij}(m+n)$ is an increasing list of the remaining numbers.

For any sequence of one-electron wave functions one can write

$$\frac{e^2}{|r_i - r_j|} v_1 * \dots * v_{m+n} = S_{\kappa_{ij}} \left\{ \left[H^{(int)} \left(v_{\kappa_{ij}(1)} * v_{\kappa_{ij}(2)} \right) \right] * v_{\kappa_{ij}(3)} * \dots * v_{\kappa_{ij}(m+n)} \right\}.$$

For this, the operator of the electron-electron interaction defined in Eq. (3) was used. Moreover, I define now

$$w_1 := x_1, \dots, w_m := x_m, w_{m+1} := y_1, \dots, w_{m+n} := y_n, \quad (8)$$

moreover the permutation " $\tau \cdot \eta$ " $\in S_{m+n}$ by

- $(\tau \cdot \eta)(l) := \tau(l), l \leq m$.
- $(\tau \cdot \eta)(l) := \eta(l - m) + m, l \geq m + 1$.

Inserting all of this into Eq. (7), the contribution

$$\begin{aligned} & \frac{1}{(m+n)!} \sum_{M \subset \{1, \dots, m+n\}: |M|=m} \sum_{\pi \in S_{m+n}} \sum_{\tau \in S_m} \sum_{\eta \in S_n} \sum_{i \leq m} \sum_{j \geq m+1} \\ & sgn(\pi_M) sgn(\pi) sgn(\tau) sgn(\eta) \\ & \left\langle Z_{\pi_M}(\tau \cdot \eta)^{-1}(\tau \cdot \eta)_{\kappa_{ij}(1)} * \dots * Z_{\pi_M}(\tau \cdot \eta)^{-1}(\tau \cdot \eta)_{\kappa_{ij}(m+n)} \right| \\ & H^{(int)} \left[w_{(\tau \cdot \eta)_{\kappa_{ij}(1)}} * w_{(\tau \cdot \eta)_{\kappa_{ij}(2)}} \right] * w_{(\tau \cdot \eta)_{\kappa_{ij}(3)}} * \dots * w_{(\tau \cdot \eta)_{\kappa_{ij}(m+n)}} \rangle \end{aligned} \quad (9)$$

of the electron-electron interaction to the matrix element is obtained. The fact that the operators $S_{\pi'}$ conserve the scalar product, $\langle S_{\pi'} \psi | S_{\pi'} \varphi \rangle = \langle \psi | \varphi \rangle$, and the relation $S_{\pi'} S_{\pi''} = S_{\pi' \pi''}$ were used for this. (In particular: $S_{\pi'}^{-1} = S_{\pi'^{-1}}$.)

For all $1 \leq i_0 \leq m, m+1 \leq j_0 \leq m+n$ and $f_0, g_0 \in \{1, \dots, m+n\}, f_0 \neq g_0$, I define the set $\Sigma_{i_0 j_0}^{f_0 g_0}$ as the set of all tuples

$$(M, \pi, \tau, \eta, (i, j))$$

with the property:

$$\begin{aligned} (\tau \cdot \eta)_{\kappa_{ij}(1)} &= i_0, \\ (\tau \cdot \eta)_{\kappa_{ij}(2)} &= j_0, \\ \pi \pi_M(\tau \cdot \eta)^{-1}(i_0) &= f_0, \\ \pi \pi_M(\tau \cdot \eta)^{-1}(j_0) &= g_0. \end{aligned}$$

The set of all tuples $(M, \pi, \tau, \eta, (i, j))$ over which the sum goes is the disjoint union of the sets $\Sigma_{i_0 j_0}^{f_0 g_0}$. The sum (9) turns into

$$\sum_{(i_0, j_0, f_0, g_0)} \sum_{(M, \pi, \tau, \eta, (i, j)) \in \Sigma_{i_0 j_0}^{f_0 g_0}} \frac{\text{sgn}(\pi \pi_M(\tau \cdot \eta)^{-1})}{(m+n)!} \langle z_{f_0} * z_{g_0} | H^{(int)} [w_{i_0} * w_{j_0}] \rangle \prod_{l \neq i_0, j_0} \langle z_{\pi \pi_M(\tau \cdot \eta)^{-1}(l)} | w_l \rangle. \quad (10)$$

There is at most one permutation " $\pi_{i_0 j_0}^{f_0 g_0}$ " $\in S_{m+n}$ with the property that the product

$$\prod_{l \neq i_0, j_0} \langle z_{\pi_{i_0 j_0}^{f_0 g_0}(l)} | w_l \rangle \quad (11)$$

is nonzero and with the property that

$$\pi_{i_0 j_0}^{f_0 g_0}(i_0) = f_0, \quad \pi_{i_0 j_0}^{f_0 g_0}(j_0) = g_0.$$

The value of the product is one in this case. If there is a permutation $\pi_{i_0 j_0}^{f_0 g_0}$ with the demanded properties, then the inner sum of expression (10) turns into

$$\text{sgn}(\pi_{i_0, j_0}^{f_0, g_0}) \langle z_{f_0} * z_{g_0} | H^{(int)} [w_{i_0} * w_{j_0}] \rangle,$$

since the number of tuples $(M, \pi, \tau, \eta, (i, j))$ in $\Sigma_{i_0 j_0}^{f_0 g_0}$ with the property $\pi \pi_M(\tau \cdot \eta)^{-1} = \pi_{i_0 j_0}^{f_0 g_0}$ is then $(m+n)!$. Swapping the position of f_0 and g_0 has the effect that the sign switches, so one obtains for $f_0 < g_0$ the equality

$$\sum_{(M, \pi, \tau, \eta, (i, j)) \in \Sigma_{i_0 j_0}^{f_0 g_0} \cup \Sigma_{i_0 j_0}^{g_0 f_0}} \frac{\text{sgn}(\pi \pi_M(\tau \cdot \eta)^{-1})}{(m+n)!} \langle z_{f_0} * z_{g_0} | H^{(int)} [w_{i_0} * w_{j_0}] \rangle \prod_{l \neq i_0, j_0} \langle z_{\pi \pi_M(\tau \cdot \eta)^{-1}(l)} | w_l \rangle = \text{sgn}(\pi_{i_0 j_0}^{f_0 g_0}) \langle z_{f_0} \otimes z_{g_0} | H^{(int)} [w_{i_0} \otimes w_{j_0}] \rangle \quad (12)$$

in case there is a permutation $\pi_{i_0 j_0}^{f_0 g_0}$ with the demanded properties (11).

The sign can be represented as

$$\text{sgn}(\pi_{i_0 j_0}^{f_0 g_0}) = \langle z_1 \otimes \dots \otimes z_{m+n} | c_{z_{f_0}}^\dagger c_{z_{g_0}}^\dagger c_{w_{j_0}} c_{w_{i_0}} [w_1 \otimes \dots \otimes w_{m+n}] \rangle.$$

The equality (12) can be rewritten as

$$\sum_{(M, \pi, \tau, \eta, (i, j)) \in \Sigma_{i_0 j_0}^{f_0 g_0} \cup \Sigma_{i_0 j_0}^{g_0 f_0}} \frac{\text{sgn}(\pi \pi_M(\tau \cdot \eta)^{-1})}{(m+n)!} \langle z_{f_0} * z_{g_0} | H^{(int)} [w_{i_0} * w_{j_0}] \rangle \prod_{l \neq i_0, j_0} \langle z_{\pi \pi_M(\tau \cdot \eta)^{-1}(l)} | w_l \rangle = \langle z_1 \otimes \dots \otimes z_{m+n} | \langle z_{f_0} \otimes z_{g_0} | H^{(int)} [w_{i_0} \otimes w_{j_0}] \rangle c_{z_{f_0}}^\dagger c_{z_{g_0}}^\dagger c_{w_{j_0}} c_{w_{i_0}} [w_1 \otimes \dots \otimes w_{m+n}] \rangle.$$

Written in this way, the equality is correct for all $1 \leq i_0 \leq m, m+1 \leq j_0 \leq m+n$ and all $1 \leq f_0 < g_0 \leq m+n$, no matter whether a permutation with the properties (11) exists. The sum (9) (= (10)) turns into

$$\langle z_1 \otimes \dots \otimes z_{m+n} | \sum_{i=1}^m \sum_{j=m+1}^{m+n} \sum_{1 \leq f < g \leq m+n} \langle z_f \otimes z_g | H^{(int)} [w_i \otimes w_j] \rangle \\ c_{z_f}^\dagger c_{z_g}^\dagger c_{w_j} c_{w_i} [w_1 \otimes \dots \otimes w_{m+n}] \rangle.$$

Going back to Eq. (7), one can write the contribution of the electron-electron interaction to the matrix element

$$\langle z_1 \otimes \dots \otimes z_{m+n} | H_T [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle$$

as

$$\langle z_1 \otimes \dots \otimes z_{m+n} | \sum_{i=1}^m \sum_{j=1}^n \sum_{1 \leq f < g \leq m+n} \langle z_f \otimes z_g | H^{(int)} [x_i \otimes y_j] \rangle \\ c_{z_f}^\dagger c_{z_g}^\dagger c_{y_j} c_{x_i} [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle \\ = \langle z_1 \otimes \dots \otimes z_{m+n} | H_T^{(int)} [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle,$$

where I used the definition

$$H_T^{(int)} := \sum_{\alpha, \alpha' \in R} \sum_{\beta, \beta' \in Q} \langle \alpha' \otimes \beta' | H^{(int)} \alpha \otimes \beta \rangle c_{\alpha'}^\dagger c_{\beta'}^\dagger c_{\beta} c_{\alpha}. \quad (13)$$

$H_T^{(int)}$ is a hermitian operator and is the contribution of the electron-electron interaction to the total tunneling Hamiltonian.

Remark:

$H_T^{(int)}$ has the alternative representation

$$H_T^{(int)} = 1/2 \sum_{\alpha \in R} \sum_{\beta \in Q} \sum_{\gamma, \delta \in R \cup Q: \gamma \neq \delta} \langle \gamma \otimes \delta | H^{(int)} \alpha \otimes \beta \rangle c_{\gamma}^\dagger c_{\delta}^\dagger c_{\beta} c_{\alpha}.$$

To verify this, one has to show that in case $\gamma \in R$ and $\delta \in R$ the matrix element

$$\langle \gamma \otimes \delta | H^{(int)} \alpha \otimes \beta \rangle$$

vanishes. One writes this as

$$\langle [(H^{(int)} - H^R) + H^R] \gamma \otimes \delta | \alpha \otimes \beta \rangle$$

and uses that $H^R(\gamma \otimes \delta) \in \overline{V(Q^\perp)}$ according to the complementarity-condition (4). Because $\beta \in Q$, the contribution of H^R vanishes. A close look and another application of the complementarity yield that also the contribution of $H^{(int)} - H^R$ vanishes.

6.2. Contribution of the potentials to H_T

Next, the contribution of $T_{m,n}^{(Q)}$ to the matrix element of Eq. (7) is determined. For this I assume $m \geq 1$ and write in the same way as in the previous subsection (Eq. 8):

$$x_{\tau(1)} * \dots * x_{\tau(m)} * y_{\eta(1)} * \dots * y_{\eta(n)} = w_{(\tau \cdot \eta)(1)} * \dots * w_{(\tau \cdot \eta)(1)}.$$

In analogy to the previous subsection, one can write for any $1 \leq i \leq m$ and any sequence v_1, \dots, v_{m+n} of one-electron wave functions

$$V^Q(r_i) [v_1 * \dots * v_{m+n}] = S_{\kappa_i} \left[(V^Q(r) v_{\kappa_i(1)}) * v_{\kappa_i(1)} * \dots * v_{\kappa_i(m+n)} \right],$$

where the permutation $\kappa_i \in S_{m+n}$, which is defined by the conditions

- $\kappa_i(1) = i$,
- $\kappa_i(2), \dots, \kappa_i(m+n)$ is an increasing (arbitrary) list of the remaining numbers $\neq i$,

was used. One obtains the contribution

$$\sum_{M, \pi, \tau, \eta} \sum_{i=1}^m \frac{\text{sgn}(\pi \pi_M (\tau \cdot \eta)^{-1})}{(m+n)!} \langle z_{\pi \pi_M (\tau \cdot \eta)^{-1} (\tau \cdot \eta) \kappa_i(1)} | V^Q(r) w_{(\tau \cdot \eta) \kappa_i(1)} \rangle \prod_{l=2}^{m+n} \langle z_{\pi \pi_M (\tau \cdot \eta)^{-1} (\tau \cdot \eta) \kappa_i(l)} | w_{(\tau \cdot \eta) \kappa_i(l)} \rangle$$

of the potential V^Q to the matrix element (7). For every $1 \leq i_0 \leq m$ and every $1 \leq f_0 \leq m+n$ I define the set $\Sigma_{i_0}^{f_0}$ as the set of all tuples

$$(M, \pi, \tau, \eta, i)$$

with the property that

$$\begin{aligned} (\tau \cdot \eta) \kappa_i(1) &= i_0, \\ \pi \pi_M \kappa_i(1) &= f_0. \end{aligned}$$

The set of all tuples over which the sum goes is the disjoint union of the sets $\Sigma_{i_0}^{f_0}$. Thus, the sum can be rewritten as

$$\sum_{i_0, f_0} \sum_{(M, \pi, \tau, \eta, i) \in \Sigma_{i_0}^{f_0}} \frac{\text{sgn}(\pi \pi_M (\tau \cdot \eta)^{-1})}{(m+n)!} \langle z_{f_0} | V^Q(r) w_{i_0} \rangle \prod_{l \neq i_0} \langle z_{\pi \pi_M (\tau \cdot \eta)^{-1} (l)} | w_l \rangle.$$

For fixed i_0, f_0 , there is at most one permutation “ $\pi_{i_0}^{f_0}$ ” with the properties

- $\prod_{l \neq i_0} \langle z_{\pi_{i_0}^{f_0}(l)} | w_l \rangle \neq 0$
- $\pi_{i_0}^{f_0}(i_0) = f_0$.

If there is such a permutation, then the number of all tuples $(M, \pi, \tau, \eta, i) \in \Sigma_{i_0}^{f_0}$ with the property that

$$\pi \pi_M (\tau \cdot \eta)^{-1} = \pi_{i_0}^{f_0}$$

is $(m+n)!$. The inner sum has in this case the value

$$\begin{aligned} & \text{sgn}(\pi_{i_0}^{f_0}) \langle z_{f_0} | V^Q(r) w_{i_0} \rangle \\ &= \langle z_1 \otimes \dots \otimes z_{m+n} | \langle z_{f_0} | V^Q(r) w_{i_0} \rangle c_{z_{f_0}}^\dagger c_{w_{i_0}} (w_1 \otimes \dots \otimes w_{m+n}) \rangle. \end{aligned}$$

The representation of the inner sum by the second line is correct even in the case that there is *no* permutation with the properties of $\pi_{i_0}^{f_0}$. Thus, the contribution of the potential V^Q to the matrix element of Eq. (7),

$$\langle z_1 \otimes \dots \otimes z_{m+n} | H_T [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle,$$

is

$$\begin{aligned} & \langle z_1 \otimes \dots \otimes z_{m+n} | \\ & \sum_{i=1}^m \sum_{f=1}^{m+n} \langle z_f | V^Q(r) x_i \rangle \quad c_{z_f}^\dagger c_{x_i} \\ & [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle = \\ & \langle z_1 \otimes \dots \otimes z_{m+n} | \\ & \sum_{\alpha \in R} \sum_{\beta \in R \cup Q} \langle \beta | V^Q(r) \alpha \rangle \quad c_\beta^\dagger c_\alpha \\ & [x_1 \otimes \dots \otimes x_m \otimes y_1 \otimes \dots \otimes y_n] \rangle. \end{aligned}$$

The sum of the contributions of the potentials V^Q and V^R to the tunneling Hamiltonian is

$$\begin{aligned} H_T^{(V)} &= \sum_{S \in \{R, Q\}} \sum_{\alpha, \alpha' \in S} \langle \alpha | V^{\bar{S}}(r) \alpha' \rangle \quad c_\alpha^\dagger c_{\alpha'} \\ &+ \sum_{S \in \{R, Q\}} \sum_{\alpha \in S} \sum_{\beta \in \bar{S}} \frac{1}{2} \langle \alpha | V(r) \beta \rangle \quad c_\alpha^\dagger c_\beta. \end{aligned} \quad (14)$$

I used the letter “ S ” to denote the two sub-systems; “ \bar{S} ” is the complementary sub-system of S ; $V(r)$ is the sum of the two potentials, $V = V^R + V^Q$.

Remark:

$H_T^{(V)}$ has the alternative representation

$$H_T^{(V)} = \sum_{S \in \{R, Q\}} \sum_{\alpha \in S} \sum_{\beta \in R \cup Q} \langle \beta | V^{\bar{S}}(r) \alpha \rangle \quad c_\beta^\dagger c_\alpha.$$

To see the identity, one can use the assumed complementarity (4) and write for $\alpha \in R, \beta \in Q$:

$$\begin{aligned} \langle \alpha | V^R \beta \rangle &= \langle (H^R - c\Delta) \alpha | \beta \rangle = \langle -c\Delta \alpha | \beta \rangle \\ &= \langle \alpha | -c\Delta \beta \rangle = \langle \alpha | -(H^Q - V^Q) \beta \rangle \\ &= \langle \beta | V^Q \alpha \rangle^*, \end{aligned}$$

where I used the abbreviation $c := -\frac{\hbar^2}{2m}$.

6.3. Expression for H_T in terms of creation- and annihilation operators: Summary

The tunneling Hamiltonian, defined by Eq. (6), is the sum of the contributions of the electron-electron interaction, Eq. (13), and that of the potentials, Eq. (14):

$$H_T = \sum_{\alpha, \alpha' \in R} \sum_{\beta, \beta' \in Q} \langle \alpha' \otimes \beta' | H^{(int)} \alpha \otimes \beta \rangle \quad c_{\alpha'}^\dagger c_{\beta'}^\dagger c_\beta c_\alpha$$

$$\begin{aligned}
& + \sum_{S \in \{R, Q\}} \sum_{\alpha, \alpha' \in S} \langle \alpha | V^{\bar{S}}(r) \alpha' \rangle c_{\alpha}^{\dagger} c_{\alpha'} \\
& + \sum_{S \in \{R, Q\}} \sum_{\alpha \in S} \sum_{\beta \in \bar{S}} \frac{1}{2} \langle \alpha | V(r) \beta \rangle c_{\alpha}^{\dagger} c_{\beta}.
\end{aligned}$$

6.4. Example

I would like to illustrate a possible effect of the additional contributions $H_T^{(int)}$, Eq. (13), to the tunneling Hamiltonian. If I assume that $\alpha, \alpha' \in R, \beta, \beta' \in Q$ with

$$\begin{aligned}
\alpha(r, \sigma) &= \psi_{lk}(r) \delta_{\downarrow}(\sigma), \\
\alpha'(r, \sigma) &= \psi_{l'k'}(r) \delta_{\uparrow}(\sigma), \\
\beta(r, \sigma) &= \varphi_{\uparrow}(r) \delta_{\uparrow}(\sigma), \\
\beta'(r, \sigma) &= \varphi_{\downarrow}(r) \delta_{\downarrow}(\sigma),
\end{aligned}$$

then the corresponding contribution to the tunneling Hamiltonian reads

$$- e^2 \int \int dr dr' \frac{\varphi_{\downarrow}(r)^* \psi_{lk\downarrow}(r) \varphi_{\uparrow}(r') \psi_{l'k'\uparrow}(r')^*}{|r - r'|} c_{\alpha'}^{\dagger} c_{\beta'}^{\dagger} c_{\beta} c_{\alpha}. \quad (15)$$

The term annihilates an electron with spin “down” in the leads as well as an electron on the quantum dot with spin “up”. At the same time, it creates an electron with spin “down” on the quantum dot and an electron with spin “up” in the leads. The term represents a spin-flip process and simultaneous scattering of electrons in the leads. The coefficient which is obtained in case $l' = l$ can be expected to be larger compared to the case $l' \neq l$ (l is the lead index).

7. Outlook

By taking the reduced density matrix and applying the projection operator technique [2], it might be possible to approach the transport problem with two leads at different chemical potentials even when terms as in the example of the last subsection are included. A complete (diagrammatic) analysis of the kernels as in Ref. [10] would be desirable, but not necessary for perturbation theory of lowest order in the tunneling Hamiltonian. The terms in H_T of the form

$$\langle \alpha | V(r) \beta \rangle c_{\alpha}^{\dagger} c_{\beta}, \quad \alpha \in S, \beta \in \bar{S},$$

give rise to energy conserving single electron tunneling seen by perturbation theory of lowest order in the tunnel coupling, e.g. Ref. [10]. Analogously, one might expect that from the terms of the form of the example (15) one obtains transition rates

$$\Gamma_{ll'}(\uparrow \rightarrow \downarrow)$$

whose value is sensitive to the question whether there are electrons and holes with appropriate spins in the leads, such that the spin-flip- and scattering process obeys the energy conservation. This might have interesting consequences for the current across the quantum dot, especially if $l \neq l'$.

8. Conclusions

I considered the Hamiltonian of an electronic system which consists of two weakly interacting sub-systems. The starting point was the many-electron Hamiltonian obtained from the Born-Oppenheimer approximation. Moreover, it was assumed that the wave functions of the states of the composite system can be constructed by the use of the wave functions of the states of the sub-systems in a natural way (antisymmetric product). The assumption of weak interaction became manifest in a “complementarity condition” (4). It turns out that the total Hamiltonian has a natural additive separation into three contributions: For each of the sub-systems one obtains a contribution which is essentially given by the Hamiltonian of the corresponding sub-system.

The contribution which expresses the interaction is called tunneling Hamiltonian. An analysis of it showed that it can be represented in a natural way in terms of annihilation- and creation operators. The contributions to the tunneling Hamiltonian are classified according to their origin: One kind of terms is caused by the electron-electron interaction, while another kind of terms is due to the interaction of the positive nuclei and the electrons.

The considerations are very general: The inner electronic structure of the sub-systems was not relevant. Even if the electron-electron interaction can be taken into account in the sub-systems by an effective noninteracting Hamiltonian, it is still expected that in the tunneling Hamiltonian the terms caused by the electron-electron interaction appear.

In my mind and in the text I used the picture that the systems are distant and separated by vacuum. As an example, the conditions for the derivations are approximately fulfilled also in the case of impurities in a metal. The sub-systems are then the impurity and the metal. The overlap of the one-electron wave functions can be expected to be small if the level generated by the impurity is localized. Apart from the transport across a quantum dot, one possible way to see whether the spin-flip scattering processes contained in the tunneling Hamiltonian yield sensible results would be to apply them to the problem of a resistivity minimum in metals doped with magnetic impurities [4], explained first in Ref. [8] by spin-flip scattering processes. The formal similarity of the problem with the transport across quantum dots led to the prediction of the zero bias resonance known as Kondo resonance [11, 6, 9]. Spin-flip scattering processes with even a similar *formulation* as in the example (15) have been taken into account for example in Ref. [3]. The coefficients of the terms are different. Nevertheless, the qualitative behaviour of the resulting current might be expected to be similar.

9. Appendix

9.1. Separation of H into one- and two-particle operators

The total Hamiltonian, Eq. (2), with general potential $V(r)$ has the natural additive separation

$$H = H^{(int)} + H_V,$$

where $H^{(int)}$ is the contribution of the electron-electron interaction, Eq. (3), and where by “ H_V ” the operator

$$H_V = -\frac{\hbar^2}{2m}\Delta + \sum_i V(r_i)$$

is denoted. The separation is obtained from a classification into one-particle operators (H_V) and two-particle operators ($H^{(int)}$), Ref. [3]. I tried to express or verify this classification also by the use of the antisymmetric product.

By methods very similar to the ones applied in the main part of the text one obtains for the action of H_V and $H^{(int)}$ on any Slater determinant of one-electron wave functions ψ_1, \dots, ψ_N :

$$\begin{aligned} H^{(int)} [\psi_1 \otimes \dots \otimes \psi_N] &= \sum_{1 \leq f < g \leq N} \text{sgn}(\kappa_{fg}) [H^{(int)}(\psi_f \otimes \psi_g)] \otimes \\ &\quad \psi_{\kappa_{fg}(3)} \otimes \dots \otimes \psi_{\kappa_{fg}(N)}, \\ H_V [\psi_1 \otimes \dots \otimes \psi_N] &= \sum_{1 \leq f \leq N} \text{sgn}(\kappa_f) [H_V \psi_f] \otimes \\ &\quad \psi_{\kappa_f(2)} \otimes \dots \otimes \psi_{\kappa_f(N)}. \end{aligned}$$

The permutations $\kappa_f, \kappa_{fg} \in S_N$ are defined in the same way as in the main text, i.e., $\kappa_f(1) = f, \kappa_{fg}(1) = f, \kappa_{fg}(2) = g$, the rest is irrelevant.

For the action of the operators on a vector space $V(R)$ generated by an arbitrary orthonormal system R of one-electron wave functions one obtains in terms of creation- and annihilation operators:

$$\begin{aligned} H^{(int)} \psi &= \sum_{\alpha \in R} (H_V \alpha) \otimes (c_\alpha \psi), \\ H_V \psi &= \frac{1}{2} \sum_{\alpha \neq \beta} [H^{(int)}(\alpha \otimes \beta)] \otimes [c_\beta c_\alpha \psi] \end{aligned}$$

for arbitrary $\psi \in V(R)$.

If $p_{V(R)}$ is the orthonormal projection onto $V(R)$, then the operator $p_{V(R)} H = p_{V(R)} (H^{(int)} + H_V)$ has the representation

$$\begin{aligned} p_{V(R)} H &= \frac{1}{4} \sum_{\alpha, \beta, \gamma, \delta \in R} \langle \gamma \otimes \delta | H^{(int)}(\alpha \otimes \beta) \rangle c_\gamma^\dagger c_\delta^\dagger c_\beta c_\alpha \\ &\quad + \sum_{\alpha, \gamma \in R} \langle \gamma | H_V \alpha \rangle c_\gamma^\dagger c_\alpha. \end{aligned} \tag{16}$$

If the orthonormal system R is chosen as a system of eigenfunctions of the one-electron operator H_V , then the second line of Eq. (16) turns into

$$\sum_{\alpha \in R} \lambda_{\alpha} c_{\alpha}^{\dagger} c_{\alpha},$$

where λ_{α} is the eigenvalue of the eigenfunction α of H_V . The latter operator is diagonal in the Slater determinants of the one-electron wave functions in R .

The potential $V(r)$ is caused by the nuclei in the crystal. If the crystal is perfectly regular, then the potential $V(r)$ can be written as a sum of a periodic contribution and a rather slowly varying non-periodic contribution: For every $r \in \mathbb{R}^3$ one can imagine a ball with centre r and positive and fixed radius. The contribution of the nuclei *within* the ball is periodic in the lattice. The contribution of the nuclei outside this ball is slowly varying and has larger negative values in the centre compared to its values closer the fringe. Therefore, the eigenfunctions of H_V might be expected to produce an electron density which is not periodic, but rather concentrated in the centre of the crystal. This is, at least in a vague sense, inconsistent with the fact that, *if* the lattice of the nuclei is perfectly periodic, then the density of the positive charges is also periodic and *not* concentrated in the centre of the crystal. With this reasoning I would assume that it might be an *inadequate* ansatz to try to find or get close to eigenfunctions of the total Hamiltonian by using Slater determinants of eigenfunctions of H_V . Even if these Slater determinants would turn out to be good approximate eigenfunctions of H , it would seem unlikely that an eigenfunction of the final Hamiltonian (including also the nuclei) can be constructed by the use of the Slater determinants.

9.2. Hybridization

Alternatively, I wrote for the action of the Hamiltonian, Eq. (2), on an N -electron wave function ψ with arbitrary $N \geq 2$:

$$\begin{aligned} H\psi &= \sum_{1 \leq i < j \leq N} \left\{ \frac{e^2}{|r_i - r_j|} + \frac{1}{N-1} [V(r_i) + V(r_j) + c(\Delta_i + \Delta_j)] \right\} \psi \\ &=: \sum_{1 \leq i < j \leq N} H_{ij}^{(N)} \psi. \end{aligned}$$

With the definition

$$H^{(N)} := \frac{e^2}{|r_1 - r_2|} + \frac{1}{N-1} [V(r_1) + V(r_2) + c\Delta]$$

(an operator acting on two-electron wave functions only) one can represent the action of H on an arbitrary Slater determinant of N one-electron wave functions as

$$\begin{aligned} H[\psi_1 \otimes \dots \otimes \psi_N] &= \sum_{1 \leq f < g \leq N} \text{sgn}(\kappa_{fg}) [H^{(N)}(\psi_f \otimes \psi_g)] \otimes \\ &\quad \psi_{\kappa_{fg}(3)} \otimes \dots \otimes \psi_{\kappa_{fg}(N)}. \end{aligned}$$

If R is an orthonormal system of one-electron wave functions, then one obtains for $\psi \in V_N(R)$:

$$H\psi = \frac{1}{2} \sum_{\alpha, \beta \in R} [H^{(N)}(\alpha \otimes \beta)] \otimes [c_\beta c_\alpha \psi]$$

and

$$p_{V(R)} H\psi = \frac{1}{4} \sum_{\alpha, \beta, \gamma, \delta \in R} \langle \gamma \otimes \delta | H^{(N)}(\alpha \otimes \beta) \rangle \quad c_\gamma^\dagger c_\delta^\dagger c_\beta c_\alpha \quad \psi$$

The representation of the action of H in terms of the operators $H^{(N)}$ seems appealing, compared to the separation into $H^{(int)}$ and H_V . Since any antisymmetric N -electron wave function can be written as an (infinite) linear combination of Slater determinants, the description of the action of H on the space of the N -electron wave functions is *equivalent* to the description of the action of the operator $H^{(N)}$ on two-electron wave functions. The representations of H obtained in the appendix are independent of the shape of the potential $V(r)$.

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